Contributions of strong collisions in the theory of spectral lines

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Contributions of strong electron-atom collisions to shift and width of spectral lines are treated via partial summation of the three-particle T matrix. Therefore, besides the width, the shift of spectral lines may be calculated also, avoiding an often-used cutoff procedure for strong collisions. As an example, shift and width of the hydrogen Lyman-α line have been calculated.

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I. INTRODUCTION

The aim of this paper is to include strong electron-atom collisions in a recently developed many-particle approach to spectral line shapes [1–10]. Within this theory, as in many approaches to shift and broadening of spectral lines, a low-order perturbation treatment has been used for the interaction between the radiator and the perturbing electrons. However, such a treatment is allowed for weak collisions only. Dealing with strong collisions, a low-order perturbative expansion for the interaction should be avoided. This problem especially is important for the strong ion-atom interaction, but it has been shown that a perturbative treatment even for the electron-atom interaction leads to an overestimation of strong-collision contributions.

Within a semiclassical treatment of the electron-radiator collisions, a low-order perturbative expansion produces even divergent integrals for shift and width. Although it is possible to overcome these divergencies within a full quantum theory, contributions of strong electron-atom collisions will be overestimated further on [9,10]. Therefore, in earlier papers [9,10] a simple cutoff procedure as proposed by Griem [11,12] has been applied for strong collisions. However, such a cutoff procedure is theoretically not well founded. Furthermore, the more or less unsteady choice of a cutoff parameter remains unsatisfactory. Whereas for linewidth calculations such a cutoff procedure has been proved to be successful, for the line shift a cutoff procedure is problematic [13]. Further, it remains an open question whether there are strong-collision contributions to the line shift at all. In Ref. [14] these contributions have been estimated to be about 20% of the weak-collision contributions. However, such an estimation could not be established yet.

Of course, within the unified theories [15–18] strong-collision contributions which do not overlap in time have been included. Unfortunately, due to the used no-quenching approximation, no line shifts could be calculated within this theory.

Another way to deal with strong collisions is to make use of the well-known relation between shift and width of the line and the scattering phase shifts given by Baranger [19]. Thus the problem is transformed into the calculation of phase shifts for the electron scattering at excited atomic states. In treating this problem, usually many atomic states must be included into the following close-coupling equations [20]. That is why it is hard to carry out such phase-shift calculations, especially for highly excited atomic states. Nevertheless, a few phase-shift calculations for determining shift and width, e.g., for the first hydrogen lines [21,22], have been carried out using asymptotic S-matrix elements.

As already shown in previous papers, a Green's-function approach is well suited to deal with spectral line shapes. Using the advantages of the diagram technique, one can find easily a complete set of contributing terms within a definite frame of approximations.

A first attempt to introduce strong-collision contributions within a Green's-function approach has been given by Dharma-wardana [23] via an "all-order" mass operator. However, within this one-particle Green's-function approach, instead of line shifts and linewidths only level shifts and widths have been treated. Here a two-particle Green's-function approach is applied to get tractable expressions for shift and width of spectral lines including strong-collision contributions. In Sec. II, via partial summation, a mass operator will be derived within a ladder approximation. It will be used in Sec. III to calculate shift and width for the hydrogen L-α line. A comparison with other theoretical results will be given.

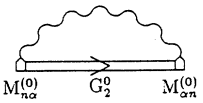
II. THEORY

Based on a Green's-function technique, a systematic approach to spectral line shapes in dense plasmas has been developed (for a short introduction see Refs. [1–10]). As a starting point, the relationship between optical properties and the dielectric function has been chosen [3,4,6]. A diagram technique has been used to select the relevant terms within the perturbative expansion. It has been shown [8] that the Green's-function approach corresponds, in principle, to the kinetic theory approach, and that the semiclassical impact approximation [11] comes out as a special approximation [6]. On the basis of this approach, shifts and widths of various spectral lines have been calculated and compared with experimental results [2,10]. Moreover, attempts have been made to describe the nonlinearity effects with respect to the density dependence of shift and broadening

of lines in dense plasmas [2,10]. So, a general quantum-statistical approach to spectral line shapes is available. However, in previous papers [1–10] only weak electron-atom collisions have been considered. The objective of this paper is to include strong electron-atom collisions into the developed theory.

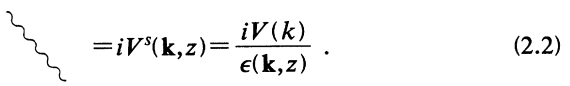
For the small plasma parameters considered here, it is allowable to decouple the ion and electron subsystems by treating the ion-electron correlation within a microfield distribution. As has been shown [1–10], the electron shift and broadening result from self-energy and vertex contributions. These can be treated in the frame of a perturbative expansion. Using a Green's-function approach it is possible to carry out this perturbation expansion in a very systematic manner. Relevant parameters for such a perturbation approach are the perturber density and the atom-perturber interaction. Due to the fact that our main concern is directed to weakly nonideal plasmas, it is reasonable to restrict the theory to modifications in the line shape which are linear in the density of the perturbing electrons.

Solving the corresponding Bethe-Salpeter equation one finds a shift of the two-particle energy compared to that of an isolated atom. It has been shown [5,7] that shifts arising from phase-space occupation due to statistical correlations and exchange are negligible. Further, shifts appear from the dynamic self-energy and a dynamically screened effective potential. Within a first-order perturbative expansion with respect to the electron-atom interaction, these terms compensate each other up to

$\Sigma_2 =$ 

(2.1)

where the electron-atom interaction is the dynamically random-phase approximation (RPA) screened Coulomb potential


$$= iV^s(\mathbf{k},z) = \frac{iV(k)}{\epsilon(\mathbf{k},z)} \, . \tag{2.2}$$

In Eq. (2.1) G_2 denotes the free two-particle propagator and

$$M^{(0)}_{n\alpha}(\mathbf{q}) = ie \int \frac{d\mathbf{p}}{(2\pi)^3} \Psi^*_n(\mathbf{p}) \{ \Psi_\alpha(\mathbf{p}) - \Psi_\alpha(\mathbf{p}+\mathbf{q}) \} \tag{2.3}$$

the isolated vertex function. (Ψ is the wave function of the isolated atom v, and e is the elementary charge.) Using the well-known relation for the screened potential (see Ref. [1])

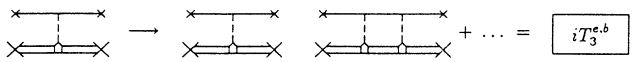

$$= iV(q) + iV(q)\Pi^{\mathrm{RPA}}(\mathbf{q},z)V^s(\mathbf{q},z) \, , \tag{2.4}$$

the self-energy in Eq. (2.1) may be split into a Hartree-Fock and a correlation term

$\Sigma_2 =$  . (2.5)

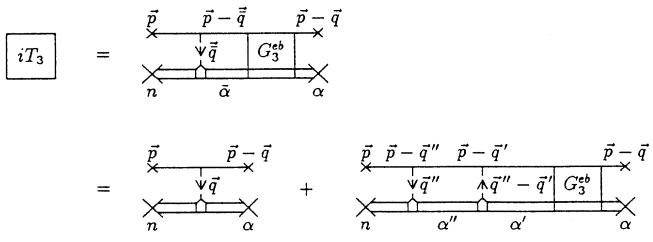
As already mentioned above, the Hartree-Fock self-energy is negligible compared to the correlation term. Therefore, only the latter will be considered further on.

In order to deal with strong collisions, in this section a ladder summation for the self-energy will be derived, avoiding a first-order Born approximation with respect to the dynamically screened interaction. For that, instead of the one static interaction line in Eq. (2.5) a three-particle T matrix T^{eb}_3 will be considered:



. (2.6)

Here a special scattering channel of the three-particle T matrix has been introduced. The T matrix T^{eb}_3 describes the full interaction between a two-particle bound state and a perturber. For this T matrix, a Dyson equation may be written



. (2.7)

Unfortunately, it is not possible to find the exact solution of Eq. (2.7). Indeed, that would correspond to an exact solution of the three-particle scattering problem.

One can find an approximative solution if only diagonal elements of the three-particle Green's function G^{eb}_3 are taken into account. That means setting $\mathbf{q}=\mathbf{q}'$ in Eq. (2.7). For isolated lines, from $\mathbf{q}=\mathbf{q}'$ it immediately follows that $\alpha=\alpha'$ holds. For hydrogen lines, the same is valid if one applies a spherical wave-function representation.

From an iteration of Eq. (2.7) it becomes obvious that this approximation is correct up to the second order with respect to the interaction potential V. This means that weak collisions are treated as before [see Eq. (2.1)] whereas the infinite sum of the selected diagrams includes strong-collision contributions. Now $T_3^{e,b}$ can be determined directly from Eq. (2.7)

$$T_3^{e,b} \approx \frac{i}{e} \frac{M_{n\alpha}^{(0)}(-\mathbf{q}) V(q)}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)} \tag{2.8}$$

with

$$A(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu) = \frac{1}{e} \sum_{\alpha''} \frac{1}{(2\pi)^3} \int d\mathbf{q}'' \frac{M_{\alpha\alpha''}^{(0)}(-\mathbf{q}'') M_{\alpha''\alpha}^{(0)}(\mathbf{q}''-\mathbf{q})}{M_{n\alpha}^{(0)}(-\mathbf{q})} \frac{V(q'')V(\mathbf{q}''-\mathbf{q})}{V(q)} \frac{1}{\Omega_\lambda + z_\nu - E_{\mathbf{p}-\mathbf{q}''} - E_{\alpha''}} . \tag{2.9}$$

Here some approximations have been applied, which were introduced already, dealing with weak collisions [1–10]. Thus, only contributions arising from charged perturbers will be taken into account, i.e., no neutral particle and no Doppler effects will be considered.

The mass operator including strong-collision contributions according to Eqs. (2.5), (2.6), and (2.9) is given by

$$\Sigma(\Omega_\lambda) = -\frac{1}{e^2} \int d\mathbf{q} \int d\mathbf{p} \frac{1}{(2\pi)^6} \frac{M_{n\alpha}^{(0)}(-\mathbf{q}) V(q) M_{\alpha n}^{(0)}(\mathbf{q})}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,E_p)} \frac{1}{(-i\beta)} \sum_\mu V^s(\mathbf{q},-\omega_\mu) G_2(\alpha_1\Omega_\lambda - \omega_\mu) \frac{i[f_e(E_p)-f_e(E_{\mathbf{p}-\mathbf{q}})]}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}} . \tag{2.10}$$

(For details see the Appendix.) If one neglects dynamic screening effects due to the electron-electron correlation (see Ref. [7–10]), the dynamic screened potential approximately may be replaced by the static Coulomb potential

$$V^s(\mathbf{q},-\omega_\mu) \approx V(q) . \tag{2.11}$$

Considering further the low-density limit, where for the Fermi distribution function $f_e \ll 1$ holds, the self-energy is given by

$$\Sigma(\Omega_\lambda) = -\frac{2}{e^2} \sum_\alpha \int d\mathbf{q} \int d\mathbf{p} \frac{1}{(2\pi)^6} V^2(q) f_e(E_p) \times \frac{|M_{n\alpha}(\mathbf{q})|^2}{E_\alpha^0 - \Omega_\lambda + E_{\mathbf{p}-\mathbf{q}} - E_p} \times [1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,E_p)]^{-1} . \tag{2.12}$$

Equation (2.12) has the same structure as the self-energy within a second-order Born approximation given in Refs. [1–10]. The only difference is the correction factor $[1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,E_p)]^{-1}$, which depends on both the momentum $\mathbf{p}$ and the transition momentum $\mathbf{q}$. That is why the $\mathbf{p}$ integration may not be carried out analytically as it could be done within the Born approximation. Whereas for weak collisions (small momentum transfers q) the correction term $iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,E_p)$ is small compared to unity, a remarkable correction of the Born approximation results for the case of strong collisions.

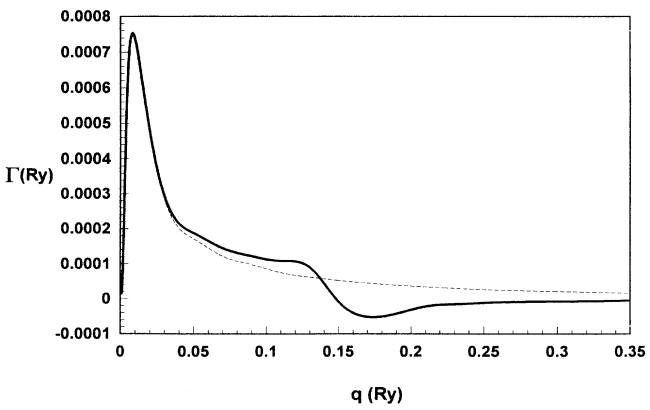


FIG. 1. q integrand for the width of the central Ly-α component ($211 \rightarrow 100$). — — —, second-order Born approximation; ——, this paper, including strong collision contributions.

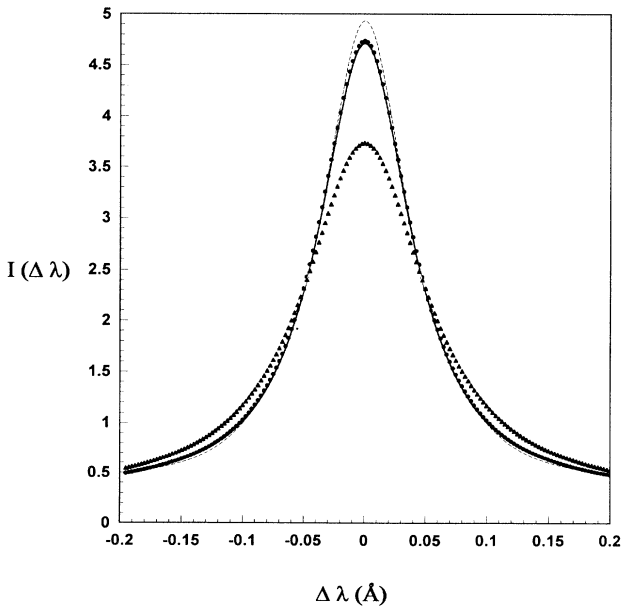


FIG. 2. Theoretical profiles of the hydrogen L-α line for $n_e = 2\times10^{17}$ cm^{-3}, $T = 13\,200$ K. The ions are treated as static perturbers using Hooper's microfield [25]. ——, this paper, including strong-collision contributions; · · · ·, unified theory, including time ordering [24]; ▲▲▲, profile resulting within a second-order Born approximation; — — —, Griem [11].

TABLE I. Electronic contribution to the shift of the hydrogen Ly-α line at an electron density of 10^{17} cm^{-3} and a temperature of 13 200 K.

	Shifts (mÅ)		Total shift (mÅ)
	$\Delta n \neq 0$ transitions	$\Delta n = 0$ transitions	
This paper	4.68	1.65	6.33
Griem [14]	4.75	2.20	6.95

III. RESULTS

After deriving a mass operator including strong-collision contributions in Sec. II, the shift and width of spectral lines have to be calculated now. As an example, the hydrogen Lyman-α line is chosen here because this line is much easier to calculate than all other hydrogen lines. Of course, the developed theory is not restricted to that line and may be applied also to nonhydrogen lines. The shift and width of the hydrogen Ly-α line have to be calculated according to Eq. (2.12). It has been shown that strong collisions produce a correction term to the well-known self-energy in a second-order Born approximation. Therefore, in order to investigate strong-collision contributions, the q integrand for the shift and width according to Eq. (2.12) will be compared with that resulting in a second-order Born approximation. In Fig. 1, the q integrand for the width of the central L-α component ($211 \rightarrow 100$) is to be seen. It becomes evident that the Born approximation works well for small values of q, which means for weak electron-atom collisions.

In Fig. 2, the resulting L-α profile is compared with that given within the Born approximation and with other theoretical profiles in which the ions are treated as static perturbers. The calculated line profile agrees excellently with the profile resulting within the unified theory including time ordering [24]. Keeping in mind that this profile should be considered as the more or less correct result for static ions, it has been shown that the theory presented is well suited to deal with strong-collision contributions to line broadening.

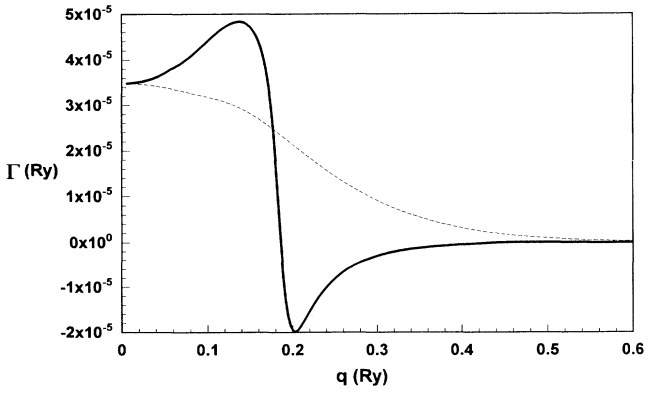


FIG. 3. q integrand for the shift of the central L-α component ($211 \rightarrow 100$). — — —, second-order Born approximation; ——, this paper, including strong-collision contributions.

Now the shift of the L-α line should be investigated. In Fig. 3, the q integrand for the shift of the central L-α component ($\Delta n = 1$ transitions) is compared with that resulting within a second-order Born approximation. It becomes evident that a cutoff procedure for the shift is much more problematic than for the width. Little changes in the cutoff parameter lead to large changes in the resulting shifts. In Table I, the calculated shift for an electron density and at a temperature of 13 200 K is compared with that given by Griem. The calculated shift due to $\Delta n \neq 0$ interactions is nearly the same as Griem's result. However, the shift due to $\Delta n = 0$ interactions is smaller than the corresponding shift given by Griem [14].

IV. CONCLUSION

Strong electron-atom collisions have been included into an earlier-developed many-particle theory to spectral line shapes. Omitting a low-order perturbative treatment for the perturber-atom interaction, a mass operator has been derived via partial summation of the three-particle T matrix.

Whereas strong-collision contributions to the width of spectral lines have already been included within the unified theory, in this paper strong-collision contributions to the line shift have also been investigated. Thus the often used cutoff procedure for strong-collision contributions introduced by Griem [11,12] could be replaced by an approach treating strong-collision contributions in a consequent manner. In order to test the developed theory, as an example, the shape of the hydrogen Lyman-α line has been calculated. The resulting line profile agrees excellently with the unified theory results [24]. The calculated shift of the L-α line is somewhat smaller than it has been given by Griem [14].

ACKNOWLEDGMENTS

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APPENDIX

According to Eqs. (2.5) and (2.6), the mass operator which includes strong collisions is given by

$$\Sigma(\Omega_\lambda)=-\frac{1}{e^2}\frac{1}{(-i\beta)^2}\sum_\nu\sum_\mu\frac{1}{(2\pi)^6}\int d\mathbf{q}\int d\mathbf{p}\,G_1(\mathbf{p},z_\nu)G_1(\mathbf{p}-\mathbf{q},z_\nu+\omega_\mu)$$
$$\times G_2(\alpha,\Omega_\lambda-\omega_\mu)\frac{M^{(0)}_{n\alpha}(-\mathbf{q})V(q)M^{(0)}_{\alpha n}(\mathbf{q})V^s(\mathbf{q},-\omega_\mu)}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}\,. \tag{A1}$$

In order to evaluate this mass operator, first one has to carry out the ν summation. The correction term A in Eq. (A1) given in Eq. (2.9) takes the form

$$A(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)\sim\frac{1}{e}\sum_{\alpha''}\frac{1}{(2\pi)^3}\int dq''\int d\Omega_{q''}\frac{F(n,\alpha'',\mathbf{q},\mathbf{q}'')}{\Omega_\lambda+z_\nu-E_{\mathbf{p}-\mathbf{q}''}-E_{\alpha''}} \tag{A2}$$

with

$$F(n,\alpha'',\mathbf{q},\mathbf{q}'')=\frac{M^{(0)}_{n\alpha''}(-\mathbf{q}'')M^{(0)}_{\alpha''\alpha}(\mathbf{q}''-\mathbf{q})}{M^{(0)}_{n\alpha}(-\mathbf{q})}\frac{V(q'')V(\mathbf{q}''-\mathbf{q})}{V(q)}q''^2\,. \tag{A3}$$

With Eq. (A2) it is possible to find a power-series expansion for the term

$$\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}=1+\sum_{j=1}^{\infty}(-1)^j\prod_{k=1}^{j}\left\{\frac{i}{e}\sum_{\alpha_k''}\int\frac{d\mathbf{q}_k''}{(2\pi)^3}\frac{F(n,\alpha_k'',\mathbf{q},\mathbf{q}_k'')}{\Omega_\lambda+z_\nu-E_{\mathbf{p}-\mathbf{q}_k''}-E_{\alpha_k''}}\right\}. \tag{A4}$$

Now, the ν summation

$$\frac{1}{-i\beta}\sum_\nu G_1(\mathbf{p},z_\nu)G_1(\mathbf{p}-\mathbf{q},z_\nu+\omega_\mu)\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}=\frac{1}{-i\beta}\sum_\nu\frac{1}{z_\nu-E_p}\frac{1}{z_\nu+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)} \tag{A5}$$

may be carried out. One arrives at

$$\frac{1}{-i\beta}\sum_\nu\frac{1}{z_\nu-E_p}\frac{1}{z_\nu+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}$$
$$=i\frac{f_e(E_p)-f(E_{\mathbf{p}-\mathbf{q}})}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}+i\sum_{j=1}^{\infty}(-1)^j\prod_{k=1}^{j}\left\{\frac{i}{e}\sum_{\alpha_k''}\int\frac{d\mathbf{q}_k''}{(2\pi)^3}\frac{F(n,\alpha_k'',\mathbf{q},\mathbf{q}_k'')}{\Omega_\lambda+E_p-E_{\mathbf{p}-\mathbf{q}_k''}-E_{\alpha_k''}}\right\}\frac{f_e(E_p)}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}$$
$$-i\sum_{j=1}^{\infty}(-1)^j\prod_{k=1}^{j}\left\{\frac{i}{e}\sum_{\alpha_k''}\int\frac{d\mathbf{q}_k''}{(2\pi)^3}\frac{F(n,\alpha_k'',\mathbf{q},\mathbf{q}_k'')}{\Omega_\lambda+E_{\mathbf{p}-\mathbf{q}}-\omega_\mu-E_{\mathbf{p}-\mathbf{q}_k''}-E_{\alpha_k''}}\right\}\frac{f_e(E_{\mathbf{p}-\mathbf{q}})}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}$$
$$+i\sum_{j=1}^{\infty}(-1)^j\prod_{k=1,k\neq l}^{j}\left\{\frac{i}{e}\sum_{\alpha_k''}\int\frac{d\mathbf{q}_k''}{(2\pi)^3}\frac{F(n,\alpha_k'',\mathbf{q},\mathbf{q}_k'')}{E_{\mathbf{p}-\mathbf{q}_l''}+E_{\alpha_l''}-E_{\mathbf{p}-\mathbf{q}_k''}-E_{\alpha_k''}}\right\}$$
$$\times\frac{f_e(E_{\mathbf{p}-\mathbf{q}_l''}+E_{\alpha_l''}-\Omega_\lambda)}{E_{\mathbf{p}-\mathbf{q}_l''}+E_{\alpha_l''}-\Omega_\lambda-E_p}\frac{1}{E_{\mathbf{p}-\mathbf{q}_l''}+E_{\alpha_l''}+\omega_\mu-\Omega_\lambda-E_{\mathbf{p}-\mathbf{q}}}\,, \tag{A6}$$

where f_e is the electron Fermi distribution function. Carrying out the μ summation now, one finds that the last two summands in Eq. (A6) result partly in terms which are proportional to the density of bound states. These terms are negligible here because only contributions due to charged perturbers are to be taken into account in this paper. Neglecting in Eq. (A6) all terms for which the μ summation results in contributions proportional to the bound state density, one arrives at

$$\frac{1}{-i\beta}\sum_{\nu}\frac{1}{z_\nu-E_p}\frac{1}{z_\nu+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}$$
$$=i\frac{f_e(E_p)-f(E_{\mathbf{p}-\mathbf{q}})}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}\left\{1+\sum_{j=1}^{\infty}(-1)^j\prod_{k=1}^{j}\frac{i}{e}\sum_{\alpha_k''}\int\frac{d\mathbf{q}_k''}{(2\pi)^3}\frac{F(n,\alpha_k'',\mathbf{q},\mathbf{q}_k'')}{\Omega_\lambda+E_p-E_{\mathbf{p}-\mathbf{q}_k''}-E_{\alpha_k''}}\right\}. \quad \text{(A7)}$$

Using Eq. (A3) now, one finds that the ν summation in Eq. (2.12) results in

$$\frac{1}{-i\beta}\sum_{\nu}G_1(\mathbf{p},z_\nu)G_1(\mathbf{p}-\mathbf{q},z_\nu+\omega_\mu)\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,z_\nu)}=i\frac{f_e(E_p)-f(E_{\mathbf{p}-\mathbf{q}})}{E_p+\omega_\mu-E_{\mathbf{p}-\mathbf{q}}}\frac{1}{1+iA(n,\mathbf{p},\mathbf{q},\Omega_\lambda,E_p)}. \quad \text{(A8)}$$

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